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Coherent states for the anharmonic oscillator and classical phase space trajectories

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Abstract Unique set of coherent states for the anharmonic oscillator is obtained by requiring i. under the quantum mechanical time evolution a coherent state evolves into another, governed by trajectory in the classical phase space (of a related hamiltonian); ii. the resolution of identity involves exactly the classical phase space measure.The rules are invariant under unitary transformations of the quantum theory and canonical transformations of the classical theory. The states are almost, but not quite, minimal uncertainty wave packets. The construction can be generalized to quantum versions of integrable classical theories.

Coherent states for the quantum harmonic oscillator are defined by,

$$|z) \;=\; e^{-\bar{z}z/2}\sum_0^\infty \frac{z^n}{\sqrt{n!}}|n> \tag{1}$$

They were constructed by Schrödinger [1] as quantum states which have close relation to classical dynamics: A.Expectation values $\hat{q}$ and $\hat{p}$ of position and momentum operators in the state $|z)$ are related to the label z by

$$z \;=\; \sqrt{\frac{\omega}{2\hbar}}q + i\sqrt{\frac{1}{2\hbar\omega}}p \tag{2}$$

Altenatively this may be viewed as providing an one-to-one correspondence between the coherent states and the classical phase space. B.Also a coherent state evolves into another coherent state under time evolution with the label z following the classical trajectory:

$$|z) \;\rightarrow\; |z(t)),\; z(t) = ze^{-i\omega t} \tag{3}$$

Coherent states have since been rediscovered and found relevant in different contexts [2, 3].There are also generalizations of the concept for some other quantum systems [2, 4, 3].These generalizations are mostly based on certain other features of the 'canonical' coherent states defined above. i.They are minimum uncertainty states of position and momentum. ii.They are eigenstates of the non-Hermitian annihilation operator. iii.They are obtained by the action of an element of the Heisenberg group on the fiducial state $|0>$. iv.They provide a representation of the Hilbert space by entire functions.

The original motivation of Schrödinger of making contact with classical dynamics has become very relevant through experimental studies [5] of microwave ionization of hydrogen Rydberg states and through manifestations of classical chaos in quantum mechanics [6].In this context there are many proposals for coherent states. (Ref. [7] and references therein.) In particular Klauder [7] has proposed coherent states for the hydrogen atom by requiring its evolution into another coherent state.However the coefficients are largely left unspecified or are fixed by requiring minimal uncertainty. Relation to classical phase space or dynamics is not imposed.

Here we propose a set of rules that provide a unique set coherent states for the quantum anharmonic oscillator, one which has exact relation to the classical phase space and dynamics and a precise semi-classical connection.Our

rules are invariant under unitary transformations of the quantum theory and canonical transformations of the classical theory. Our criteria can be readily applied to other quantum systems.In particular, they provide a unique set of coefficients for the hydrogen atom. This and its relation to the earlier proposals will considered elsewhere.

For our construction, in addition to the properties A and B, the following properties of the canonical coherent states are crucial.

C.Semiclassical limit: The coefficients peak at the value n where $d/dn(nln|z|^2 - lnn!) = 0$. This gives the largest coefficient to be the one corresponding to $n \approx |z|^2$.(Width of the peak is $O(|z|)$).

Consider Bohr-Sommerfeld quantization condition $\oint pdq = (n+1/2)h$.Now,

$$\int_0^T p\dot{q}dt = \frac{1}{2}a^2\omega^2 T \tag{4}$$

where the amplitude $a = \omega^{-1}\sqrt{p^2 + \omega^2 q^2}$. Thus $(p^2+\omega^2 q^2)/2 = (n+1/2)\hbar\omega$. With the identification Eqn. 2, this is precisely where the coefficients peak. Therefore the relation to the classical phase space is more than just an identification of the labels. For large $|z|$, the canonical coherent state is dominated by stationary states near the one corresponding to the Bohr quantization of the corresponding classical orbit.

It is to be noted that the properties A and B would be true with any choice of the n-dependence of the coefficients. The property C fixes the n-dependence atleast asymptotically.

D.Resolution of the identity: We have,

$$\mathbf{1} \quad = \quad \int \frac{d^2 z}{\pi} |z)(z| \tag{5}$$

Now with the identification Eqn.2, $\pi^{-1}d^2 z = h^{-1}dpdq$ is the canonical measure on the classical phase space measured in units of the Planck's constant.z and n dependence of the coefficients as in Eqn. 1 is crucial for this simple interpretation. For instance, if we had

$$|z) \quad = \quad \sum_0^\infty c_n(r) e^{-in\theta}|n>, \ \sum_0^\infty |c_n(r)|^2 = 1 \tag{6}$$

where $z = rexp(-i\theta)$, then properties A and B would be true and C could also be valid for a wide choice of $c_n(r)$ (for e.g., any monotonically increasing

function of $r^n/\sqrt{n!}$).States $|z)$ would still provide an (over)complete set of states and therefore a resolution of the identity would be still possible.Now,

$$\int_0^{2\pi} \frac{d\theta}{2\pi} |z)(z| = \sum_0^{\infty} |c_n(r)|^2 |n >< n| \tag{7}$$

For a resolution of the identity we need a measure $d\mu(r)$ such that

$$\int d\mu(r) |c_n(r)|^2 = 1 \tag{8}$$

As has been emphasised by Klauder [7],There are many choices of $c_n(r)$ meeting this requirement. But the measure $\int d\mu(r) d\theta/\pi$ would not have a simple interpretation as the canonical measure on the classical phase space.The set of coefficients of the canonical coherent states are unique in this respect.

We use the ingredients A-D to construct coherent states for other quantum systems.We first consider the Hamiltonian

$$H = (a^* a + 1/2)\hbar\omega + \lambda((a^* a + 1/2)\hbar\omega)^2 \tag{9}$$

which is already in the diagonal form.Relevance to the anharmonic oscillator will become clear later.Corresponding classical Hamiltonian is $H((p^2 + \omega^2 q^2)/2)$ obtained by the replacement

$$(a^* a + 1/2)\hbar\omega = (p^2 + \omega^2 q^2)/2 \tag{10}$$

Classical equations of motion are

$$\dot{q} = H' p, \ \dot{p} = -\omega^2 H' q \tag{11}$$

where $H'(y) = dH(y)/dy$ is a constant of motion related to the amplitude or energy.The classical trajectories in the phase space are circles as in the harmonic case but the frequency $\Omega = H'\omega$ depends on the amplitude. Classical trajectories are

$$q = R \, cos(\Theta + \omega H' t), \, p = -R\omega \, sin(\Theta + \omega H' t) \tag{12}$$

where the amplitude $R = R(t) = \omega^{-1}\sqrt{p(t)^2 + \omega^2 q(t)^2}$ is a constant of motion. We may regard $R(t)$ as the action variable and $\Theta(t) = tan^{-1}(p(t)/(\omega q(t)))$ as the conjugate angle variable.Their time evolution is given by

$$R(t) = constant, \, \Theta(t) = \Theta + \omega H' t, \tag{13}$$

In order to construct the coherent states now we now use R and Θ to label the classical phase space:

$$|R, \Theta) \;=\; \sum_{0}^{\infty} c_n(R, \Theta)|n>, \tag{14}$$

where the energy eigenstates $|n>$ are now the same as in the harmonic case, but have different energy eigenvalues as the Hamiltonian is different. We now apply our criteria A-D for the coefficients $c_n(R, \Theta)$. Under time evolution, $|n> \rightarrow exp(-iE_n t/\hbar)|n>$ where E_n are the exact eigenvalues of H obtained by replacing a^*a by n in Eqn. 9. In order that a coherent state evolve into a coherent state the only possible choice is

$$|R, \Theta) \;=\; \sum_{0}^{\infty} c_n(R) exp(-iE_n \frac{\Theta}{\hbar\omega H'})|n> \tag{15}$$

This brings home the crucial difference with the harmonic case. The angle variable Θ in the classical phase space is periodic with range $[0, 2\pi)$.But the quantum mechanical state $|R, \Theta)$ defined above is not periodic in Θ when the energies E_n are incommensurate.This is unavoidable once we impose criterion B as has been noted by Klauder [7].Thus the label Θ has to be extended to the covering space, $\Theta\epsilon(-\infty, \infty)$. In spite of this the relation to the classical phase space with Θ as the angle variable survives, as seen below.For an observable O, time dependence of the expectation value is $< O(t) >= \sum < m|O|n > exp(-i(E_n - E_m)t/\hbar)$ which can never be periodic in case the energy levels are incommensurate with each other and the state is not stationary. Instead, it is an *almost periodic function* [8] of time. There is no possibility of relating it to periodic orbits except in the sense considered above and therefore this feature need not be regarded as undesirable.

We now apply criterion C. The Bohr quantization gives

$$\frac{1}{2} R^2 \omega^2 H' T = nh \tag{16}$$

Now the period $T = 2\pi(\omega H')^{-1}$.Therefore we get the quantization condition $(p^2 + \omega^2 q^2)/2 = (n + 1/2)\hbar\omega$ exactly as in the harmonic case with $a^*a \rightarrow n$ as is to be expected.

For criterion C we require the coefficients $c_n(R)$ to peak at $n \approx R^2$.Same choice as in the harmonic oscillator suffices:$c_n(R) = R^n/\sqrt{n!}$.However, the choice is not unique at this stage.

We now apply criterion D.As $|R, \Theta)$ is not periodic in Θ we cannot simply integrate over the range $[0, 2\pi)$ in order to resolve the identity.In order to retain the interpretation of the canonical phase space measure, we will consider averaging over infinitely many classical orbits:

$$[\int_{-\pi}^{\pi}]\frac{d\Theta}{2\pi} = lim_N \rightarrow \infty \;\; \frac{1}{N}\int_{-\pi N}^{\pi N}\frac{d\Theta}{2\pi} \tag{17}$$

We now have

$$[\int_{-\pi}^{\pi}]\frac{d\Theta}{2\pi}e^{-i(E_n-E_m)\Theta} = \delta_{nm} \tag{18}$$

Therefore

$$[\int_{-\pi}^{\pi}]|R, \Theta)(R, \Theta| = \sum_{0}^{\infty}|c_n(R)|^2|n >< n| \tag{19}$$

This shows that the choice also satisfies the criterion D.

$$\mathbf{1} \;\; = \;\; \int_0^{\infty}\frac{dR^2}{2}[\int]\frac{d\Theta}{\pi}|R, \Theta)(R, \Theta| \tag{20}$$

with $(2\pi)^{-1}dR^2d\Theta = h^{-1}dpdq$. Thus we have got a unique set of coherent states closely related to the classical phase space and time evolution.

The form of Eqn. 15 suggests a new choice of conjugate variables with $\tau = (\omega H')^{-1}\Theta = (\omega H')^{-1}tan^{-1}(p/(\omega q))$ as the new angle variable.The conjugate action variable is just the Hamiltonian H as in the Hamilton-Jacobi theory. Under time evolution we have,

$$H = constant, \; \tau \rightarrow \tau + t \tag{21}$$

τ is the time variable promoted to a dynamical degree of freedom.As this is a canonical set, the phase space measure is simply $dHd\tau$.The range of τ is $[0, 2\pi/(\omega H'))$ (one period), and not just $[0, 2\pi)$, and therefore depends on the value of H.We could label the coherent states $|R, \Theta)$ by $|H, \tau)$ as well, with the understanding that R in $c_n(R)$ is reexpressed in terms of H. The coefficients ofcourse would have different forms for different Hamiltonians, and not have the simple form as when written in terms of the R variable. On the other hand, the phase has a simple form $exp(-iE_n\tau/\hbar)$.

We now consider the anharmonic oscillator

$$\hat{\mathbf{H}} = \frac{1}{2}(\hat{P}^2 + \omega^2\hat{Q}^2 + \lambda\hat{Q}^4) \tag{22}$$

When $\lambda \neq 0$ the orbits in the phase space are closed but not circles and has an amplitude dependent frequency. By a canonical transformation we may pass to the action angle variables.Now the orbits are circular.In the quantum mechanical case this procedure corresponds to a unitatry transformation that diagonalises the Hamiltonian:

$$\hat{\mathbf{H}}(\hat{P}, \hat{Q}) = \hat{H}((\hat{p}^2 + \hat{q}^2)/2); \tag{23}$$

$$\hat{P}(\hat{p}, \hat{q}) = \hat{U}\hat{p}\hat{U}^*, \quad \hat{Q}(\hat{p}, \hat{q}) = \hat{U}\hat{q}\hat{U}^* \tag{24}$$

$H(y)$ is a monotonic function of the argument such that $H(y = (n+1/2)\hbar) = E_n$, the energy levels. In terms of the creation and annihilation operators a^*, a for p, q, a formal expression for the diagonalised form is $H = \sum_0^\infty H_n a^{*n} a^n$, where the coefficients H_n are related to the energy levels E_n *via*

$$H_n = \frac{1}{n!}\frac{d^n}{dy^n}(e^{-y}\sum_0^\infty \frac{E_m}{m!}y^m)|_{y=0} \tag{25}$$

For the Hamiltonian H we may simply apply our construction of the coherent states.These will also be the coherent states of the anharmonic oscillator.$|n>$ are now the energy eigenstates of the anharmonic oscillator, labelled by non-negetive integers. The coherent states are labeled by the conjugate pair R and Θ (or equivalently, H and τ) defined in terms of the pair p, q as before. We would like to label it by the conjugate pair P and Q in the Hamiltonian Eqn. 22.But there would be no canonical transformation of the classical theory which takes the Hamiltonian $H((p^2 + q^2)/2)$ to the Hamiltonian $\mathbf{H}(P, Q)$, Eqn.22. Only in the region $(p^2 + q^2) >> \hbar$ would the two be related by a canonical transformation. We could in any case choose the new conjugate pair $\mathcal{P}, \mathcal{Q}$ to get the Hamiltonian in the form $\mathcal{H} = \mathcal{P}^2/2 + u(\mathcal{Q})$ with a new potential $u(\mathcal{Q})$.In the present case it is easy to give the formal method for obtaining the new potential $u(\mathcal{Q})$ and the relationship between the pairs H, τ and $\mathcal{P}, \mathcal{Q}$. We need to only match energies and periods of the orbits of the two systems.Explicitly,

$$\frac{\pi}{H'} = 2\int_0^{\mathcal{H}} du \frac{d\mathcal{Q}/du}{\sqrt{2(H-u)}} \tag{26}$$

matches the periods of an orbit in terms of the two sets of variables.This may be viewed as an implicit functional equation for $\mathcal{Q}$ as a function of u or equivalently, the new potential $u(\mathcal{Q})$ in terms of H.Once $u(\mathcal{Q})$ is known, $\mathcal{P}$ can be obtained from

$$H = \frac{1}{2}\mathcal{P}^2 + u(\mathcal{Q}) \tag{27}$$

which is a matching of the energies in the two variables. Finally $\mathcal{Q}$ is related to the old pair H, τ by

$$\tau = \int_0^{\mathcal{Q}} \frac{d\mathcal{Q}}{\sqrt{2(H - u(\mathcal{Q}))}} \tag{28}$$

which uses the interpretation of τ as the canonical variable corresponding to time. When labelled in terms of $\mathcal{P}$ and $\mathcal{Q}$, the time evolution of the coherent states will be given by the classical trajectories of the Hamiltonian with the potential $u(\mathcal{Q})$ and not of the anharmonic oscillator we started with. τ would be a multivalued function of $\mathcal{P}$ and $\mathcal{Q}$, and it is important that this multivaluedness be retained in the coherent state written in terms of $\mathcal{P}$ and $\mathcal{Q}$.

Canonical coherent states are minimal uncertainty wave packets with the expectation value of position and momentum directly given by the imaginary and the real part respectively of the label z. We now consider these issues for our coherent states. We first discuss the case of the Hamiltonian Eqn. 9.When the energy levels are incommensurate relative to each other, these coherent states can no longer be eigenfunctions of the annihilation operator a. We have,

$$a|R,\Theta) \;\; = \;\; e^{-R^2}\sum_0^\infty \frac{R^{n+1}}{\sqrt{n!}} exp(-i(E_{n+1}-E_n)\frac{\Theta}{\hbar H'}) \tag{29}$$

Only for the harmonic oscillator, we get $R\ exp(-i\Theta)$ on the r.h.s.In the general case this is an almost periodic function of time [8].In particular the value gets arbitrarily close but does not quite repeat after an interval of time.However, for large R, the coefficients $n \approx R^2$ dominate and $(E_{n+1} - E_n) \approx \hbar H'$ for such values. Therefore $a|R,\Theta) \approx Rexp(-i\Theta)|R,\Theta)$(By this we mean $(a - Rexp(-i\Theta))|R,\Theta)$ has a small norm.) In particular this means

that expectation values of p and q in our coherent states $|R,\Theta)$ are approximately $R\ sin\Theta$ and $R\ cos\Theta$, the approximation becoming rapidly better for large R.

We now consider the spread in position and momentum and Heisenberg uncertainty for our coherent states. An explicit calculation gives, $\Delta q^2 = \hbar(2\omega)^{-1}(1+R^2 k(R,\Theta))$, where

$$\begin{aligned} k(R,\Theta) &= 2e^{-R^2}\sum_0^\infty \frac{R^{2n}}{n!}(cos\frac{(E_{n+2}-E_n)\Theta}{\hbar H'\omega} - cos(2\Theta)) \\ &\quad -4e^{-R^2}\sum_0^\infty \frac{R^{2n}}{n!}(cos\frac{(E_{n+1}-E_n)\Theta}{\hbar H'\omega} - cos\Theta) \\ &\quad \times(2+e^{-R^2}\sum_0^\infty \frac{R^{2n}}{n!}(cos\frac{(E_{n+1}-E_n)\Theta}{\hbar H'\omega} - cos\Theta) \end{aligned}$$

$k(R,\Theta) \to 0$ for $R \to \infty$.If this asymptotic falloff is faster than R^{-2}, then $\Delta q^2 \approx \hbar(2\omega)^{-1}$. In the present case an explicit asymptotic analysis can be made to justify this result.Similar results are also valid for Δp^2. In particular this means that atleast for large p^2+q^2, the coherent state is almost a minimal uncertainty wave packet, the correction being very tiny for large R.

We now argue that these properties are also valid for the observables $\hat{P},\hat{Q}$ of the anharmonic oscillator, Eqn.22.$\hat{p},\hat{q}$ are operator expressions in $\hat{P},\hat{Q}$ such that when substituted in $\hat{H}((\hat{p}^2+\hat{q}^2)/2)$ only dependence on P^2 is quadratic, Eqn.24. On the other hand, the classical variables p,q are functions of $\mathcal{P},\mathcal{Q}$ such that when substituted in the classical Hamiltonian $H((p^2+q^2)/2)$, we get $\mathcal{P}^2/2+u(\mathcal{Q})$, with only a quadratic term in $\mathcal{P}$.The two sets of functions differ only in higher orders in $\hbar$, in particular, due to ordering of operators.In the semiclassical region, of large p^2+q^2, these are neglegible. In this region the expectation values $(R,\Theta|\hat{P}|R,\Theta)$ and $(R,\Theta|\hat{Q}|R,\Theta)$ are computed by substituting the operator expressions in $\hat{p},\hat{q}$, rewriting these expressions in normal ordered form in a,a^* and simply replacing $a \to R\ exp(-i\Theta)$ and $a^* \to R\ exp(+i\Theta)$. Therefore upto terms of $O(h)$, these are same as $\mathcal{P}$ and $\mathcal{Q}$ for these values of R and Θ.Also as the canonical transformations preserve the area, the spread of the wavepacket in $\mathcal{P},\mathcal{Q})$ is the same as the spread in p,q. Thus they are *almost* minimum uncertainty states, though not exactly so. Therefore our coherent states for the anharmonic oscillator have properties of the canonical coherent states in the semiclassical region.

The coherent states we have constructed are same for Hamiltonians that are equivalent under unitary transformations. They may be labelled by any choice of conjugate variables of the classical phase space.Their properties $vis-a-vis$ classical dynamics are invariant under the choice of the conjugate variables.

Our construction uses the one parameter group associated with the time evolution crucially and is not tied to other groups such as the Heisenberg group or symmetry groups of specific Hamiltonians, such as the rigid rotator or the hydrogen atom.As such it can be used for general Hamiltonians.This will be considered elsewhere cite [9].

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